Scaling Behavior of Entanglement in Two- and Three-Dimensional Free Fermions

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Exactly solving a spinless fermionic system in two and three dimensions, we investigate the scaling behavior of the block entropy in critical and non-critical phases. The scaling of the block entropy crucially depends on the nature of the excitation spectrum of the system and on the topology of the Fermi surface. Noticeably, in the critical phases the scaling violates the area law and acquires a logarithmic correction *only* when a well defined Fermi surface exists in the system. When the area law is violated, we accurately verify a conjecture for the prefactor of the logarithmic correction, proposed by D. Gioev and I. Klich [quant-ph/0504151].

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The nature of many-body entanglement in various solid-state models has been the focus of recent interest. The motivation for this effort is two-fold. On the one side, these systems are of interest for the purpose of quantum information processing and quantum computation [1]. At a fundamental level, the study of entanglement represents a *purely quantum* way of understanding and characterizing quantum phases and quantum phase transitions in many-body physics [2, 3, 4, 5].

A striking feature of entangled states $|\Psi\rangle$ is that a *local* accurate description of such states is impossible, namely each subsystem A of the total system U can have a *finite* entropy, quantified as the von-Neumann entropy $S_A = -\mathrm{Tr}\rho_A \log_2 \rho_A$ of its reduced density matrix $\rho_A = Tr_{U\setminus A}|\Psi\rangle\langle\Psi|$, whereas the total system clearly has zero entropy. The *entropy of entanglement* S_A of the subsystem is a reliable estimate of the entanglement between the subsystem A and the rest, $U \setminus A$. Assuming that the system U corresponds to the whole universe in d dimensions, a fundamental question concerns the scaling behavior of the entropy of entanglement S_L of an hypercubic subsystem L^d (hereafter denoted as a *block*) with its size L. Indeed, such scaling probes directly the spatial range of entanglement: when the block size exceeds the characteristic length over which two sites are entangled, the block entropy should become subadditive, and scale at most as the area of the block boundaries, following a so-called *area law*: $S_L \sim L^{d-1}$. A crucial question is then if and how the scaling of the block entropy changes when the nature of the quantum many-body state evolves in a critical way by passing through a quantum phase transition, and how the characteristic spatial extent of entanglement relates to the correlation length of the system.

This question has been extensively addressed in the case of one-dimensional spin systems [5, 6, 7, 8], in chains of harmonic oscillators [9, 10] and in related conformal field theories (CFT) [11, 12]. Here it is found unambiguosly that in states with exponentially decaying (connected) correlators S_L follows the area law $S_L \sim L^0$, saturating to a finite value, whereas for critical states, displaying power-law decaying correlations, a *logarithmic correction* to the area is always present: $S_L = [(c+\bar{c})/6]\log_2 L$, where c is the central charge of the related CFT. The asymptotic value of the block entropy is found to diverge logarithmically with the correlation length, $S_\infty \sim \log_2(\xi)$, which clearly establishes the relationship between entanglement and correlations. The above picture holds true only in presence of *short-range* interactions; on the contrary, in presence of long-range interactions the divergence of the correlation length can be still accompanied by the area law [10, 13].

In higher spatial dimensions less results are available, and the general relationship between the block entropy scaling and the correlation properties of the quantum state is still unclear even for short-range interactions. In free-boson systems, it has been generally proven that the area law is satisfied for non-critical systems [10, 14]. For free-fermion systems, on the other hand, it has been proven [15, 16] that critical systems with short-range hoppings and a finite Fermi surface exhibit a logarithmic correction to the area law

$$S_L = C/3\ (\log_2 L)\ L^{d-1}. \tag{1}$$

In this paper, we investigate a general quadratic fermionic Hamiltonian both in $d = 2$ and $d = 3$. Upon tuning the Hamiltonian parameters, this model has distinct critical phases *with* and *without* a finite Fermi surface, as well as non-critical phases. The scaling behavior of the block entropy is accurately obtained through exact diagonalization. In non-critical states we find that the area law indeed holds, and we confirm that logarithmic corrections to such law are present in critical states with a finite Fermi surface, as found in Refs. 15, 16. The prefactor C of the L-dependence of S_L in Eq.(1) is found to be very accurately predicted by a formula based on the Widom conjecture [16]. On the other hand, for critical states with a Fermi surface of zero measure, we find that the corrections to the area law are either *absent* or *sublogarithmic*. This means that the relationship between entanglement and correlations in higher dimensional sys-

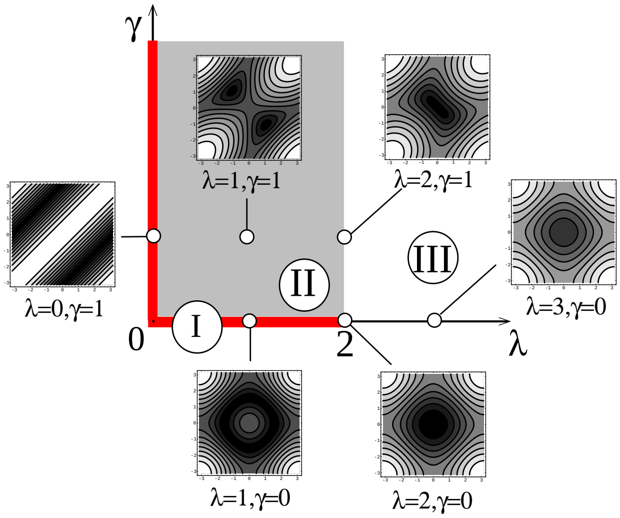

FIG. 1: Phase diagram of the model Eq.(2) for the case $d = 2$. The roman numbers for the various phases are explained in the text. Representative contour plots of the dispersion relation $\Lambda_{\boldsymbol{k}}$ are also shown. There the black areas corresponds to $\Lambda_{\boldsymbol{k}} = 0$ and the white areas to the top of the band.

tems is different than in $d = 1$, and that a crucial role is played by the geometry of the Fermi surface or, alternatively, by the density of states at the ground state energy.

We consider a bilinear spinless fermionic system on a d-dimensional hypercubic lattice with hopping and pairing between nearest-neighbor lattice sites

$$H = \sum_{\langle \boldsymbol{ij} \rangle} \left[c_{\boldsymbol{i}}^{\dagger} c_{\boldsymbol{j}} - \gamma (c_{\boldsymbol{i}}^{\dagger} c_{\boldsymbol{j}}^{\dagger} + c_{\boldsymbol{j}} c_{\boldsymbol{i}}) \right] - \sum_{\boldsymbol{i}} 2 \lambda c_{\boldsymbol{i}}^{\dagger} c_{\boldsymbol{i}}. \qquad (2)$$

λ is the chemical potential, while γ is the pairing potential. The sum of $\sum_{\langle \boldsymbol{ij} \rangle}$ extends over nearest-neighbor pairs. The above Hamiltonian is a $d > 1$ generalization of the $1d$ spinless fermionic Hamiltonian which is obtained by Jordan-Wigner transformation of the XY model in a transverse field [17]. Although in $d > 1$ the exact relationship to the XY model is lost, we can imagine the above Hamiltonian to represent the effective fermionic degrees of freedom of an interacting system with quantum-critical phases.

A more insightful expression for the Hamiltonian of Eq. (2) is obtained upon Fourier transformation to momentum space:

$$H = \sum_{\boldsymbol{k}} \left[-2 t_{\boldsymbol{k}} c_{\boldsymbol{k}}^{\dagger} c_{\boldsymbol{k}} + i \Delta_{\boldsymbol{k}} (c_{\boldsymbol{k}}^{\dagger} c_{-\boldsymbol{k}}^{\dagger} + c_{-\boldsymbol{k}} c_{\boldsymbol{k}}) \right]$$

$$t_{\boldsymbol{k}} = \lambda - \sum_{\alpha=1}^{d} \cos k_{\alpha} \qquad \Delta_{\boldsymbol{k}} = \gamma \sum_{\alpha=1}^{d} \sin k_{\alpha} \quad (3)$$

The pairing potential in $\boldsymbol{k}$-space, $\Delta_{\boldsymbol{k}}$, clearly reveals a p-wave symmetry.

This Hamiltonian can be diagonalized exactly by a Bogoliubov transformation, to give

$$H = \sum_{\boldsymbol{k}} \Lambda_{\boldsymbol{k}} f_{\boldsymbol{k}}^{+} f_{\boldsymbol{k}} \qquad \Lambda_{\boldsymbol{k}} = 2 \sqrt{t_{\boldsymbol{k}}^2 + \Delta_{\boldsymbol{k}}^2} \qquad (4)$$

Depending on the parameters γ and λ, this system has a rich phase diagram, including metallic, insulating and (p-wave) superconducting regimes, as shown in Fig. 1. The different phases are certainly distinguished by the different decay of the correlation function, which tells apart the critical from the non-critical phases. Nonetheless, a classification which turns out to be relevant for the study of entanglement is based on the features of the gapless excitation manifold $\Lambda_{\boldsymbol{k}} = 0$. Such manifold can be characterized by the *density of states* at the ground-state energy $g(0)$, and by the so-called *co-dimension* [18, 19] $\bar{d}$, defined as the dimension of $\boldsymbol{k}$-space minus the dimension of the $\Lambda_{\boldsymbol{k}} = 0$ manifold. We notice that the existence of a finite Fermi surface at zero energy implies that $\bar{d} = 1$ and $g(0) > 0$, while in absence of a finite Fermi surface we have $\bar{d} \geq 2$ and $g(0) > 0$ or $g(0) = 0$ depending on the dispersion relation $\Lambda_{\boldsymbol{k}}$ around its nodes.

According to this classification, which turns out to be relevant for the study of entanglement, we can distinguish three phases:

- *Phase I*, $\{0 \leq \lambda \leq d, \gamma = 0\}$, and $\{\lambda = 0, \gamma > 0\}$ if $d = 2$. For $\gamma = 0$, Eq. (2) reduces to a simple tight-binding model, which is in a metallic state with a $2d$-fold symmetric Fermi surface as far as $\lambda \leq d$. In $d = 2$, for $\lambda = 0$ the system is still a metal with a well defined Fermi surface, which is simply $k_x = k_y \pm \pi$, and whose symmetry is lowered by the presence of the γ term in the Hamiltonian. In this phase, $g(0) > 0$, and $\bar{d} = 1$ everywhere except at the point $\{\lambda = d, \gamma = 0\}$ where $\bar{d} = 2$.

- *Phase II*, $\{0 < \lambda \leq d, \gamma > 0\}$, and $\{\lambda = 0, \gamma > 0\}$ if $d = 3$. Away from the boundary lines of this phase, the system is in a p-wave superconducting state, with a finite pairing amplitude $\langle c_{\boldsymbol{k}}^{\dagger} c_{-\boldsymbol{k}}^{\dagger} \rangle \neq 0$. Such pairing amplitude vanishes at the boundaries of this region. The dispersion relation $\Lambda_{\boldsymbol{k}}$ has point nodes in $d = 2$ and line nodes in $d = 3$. Everywhere in this phase $g(0) = 0$ and $\bar{d} = 2$.

- *Phase III*, $\{\lambda > d\}$. In this phase the system is in an insulating state with a gap in the excitation spectrum. Here $g(0) = 0$ and $\bar{d} = d$.

This shows that, in terms of the spectral properties, the above system has *two distinct critical phases*, (*I* and *II*), which are both gapless, and a *non-critical* phase (*III*). Numerical evaluation of the correlation function through integration over the first Brillouin zone (FBZ),

$$< c_{\boldsymbol{i}}^{+} c_{\boldsymbol{j}} >= \int_{FBZ} \frac{d^d k}{(2\pi)^d} \frac{t_{\boldsymbol{k}}}{2\Lambda_{\boldsymbol{k}}} e^{i \boldsymbol{k} \cdot (\boldsymbol{i}-\boldsymbol{j})}, \qquad (5)$$

shows an expected power-law decay in the critical phases and an exponential decay in the non-critical one.

We then proceed to the evaluation of the block entropy of entanglement. The ground state of Eq.(2) is known to be a Gaussian state, whose density matrix can be expressed as the exponential of a quadratic fermion operator [20, 21]. To obtain the reduced density matrix of a L^d subsystem, Grassman algebra is needed [22]. Using a Bogoliubov transformation, the reduced density matrix ρ_L can then be written as

$$\rho_L = A\ \exp\left(-\sum_{l=1}^{L}\varepsilon_l d_l^+ d_l\right), \qquad (6)$$

where d_l^+,d_l are the new Fermi operators after the transformation, and A is a normalization constant to ensure $Tr(\rho) = 1$. The single-particle eigenvalues ε_l can be obtained from $\langle c_i^+ c_j\rangle$ and $\langle c_i^+ c_j^+\rangle$ by the following formula[21]:

$$(C - F - \tfrac{I}{2})(C + F - \tfrac{I}{2}) = \frac{1}{4}\ P\ \text{diag}\left\{\tanh^2\left(\tfrac{\varepsilon_1}{2}\right), \tanh^2\left(\tfrac{\varepsilon_2}{2}\right), ..., \tanh^2\left(\tfrac{\varepsilon_L}{2}\right)\right\} P^{-1} \qquad (7)$$

where $C_{i,j} = \langle c_i^+ c_j\rangle$ and $F_{i,j} = \langle c_i^+ c_j^+\rangle$;$P$ is the orthogonal matrix that diagonalizes the left side of the above equation. The Block entropy can then be calculated in terms of ε_l as:

$$S_L = \sum_{l=1}^{L}\left\{\ln\left[1 + \exp(-\varepsilon_l)\right] + \frac{\varepsilon_l}{\exp(\varepsilon_l) + 1}\right\} \qquad (8)$$

In $d = 1$ the above formulas reproduce the scaling of the block entropy as observed in the XY model in a transverse field [5, 6]. In $d = 2$ the phase diagram is richer, and we need to consider the various phases one by one. We begin with the critical metallic phase (I), $\gamma = 0, 0 \le \lambda < d$. For this case a logarithmic correction to the area law, $S_L = (C(\lambda)/3)(\log_2 L)L^{d-1}$ is observed for all values of λ, as shown in Fig. 2. This is in full agreement with the results of Refs.[15, 16], which predict this behavior in presence of a finite Fermi surface. More specifically, Ref. 16 also supplies us with an explicit prediction for the λ dependence of $C(\lambda)$, based on the Widom's conjecture [23], in the form

$$C(\lambda) = \frac{1}{4(2\pi)^{d-1}}\int_{\partial\Omega}\int_{\partial\Gamma(\lambda)}|n_x\cdot n_p|dS_x dS_p \qquad (9)$$

where Ω is the volume of the block normalized to one, $\Gamma(\lambda)$ is the volume enclosed by the Fermi surface, and the integration is carried over the surface of both domains. A numerical fit of the calculated asymptotic behavior of S_L through the formula $S_L = \frac{C}{3}L^{d-1}\log_2(L) + BL^{d-1} + AL^{d-2} + ...$ provides us with the exact result for the $C(\lambda)$ prefactor. In Fig. 3 the prediction of Ref. 16, Eq.(9), for the case $\{0 \le \lambda \le d, \gamma = 0\}$ is compared to our numerical results both for $d = 2$ and $d = 3$. The agreement is clearly striking. Moreover, for $\{\lambda = 0, \gamma > 0\}$ in $d = 2$ the formula Eq.(9) predicts $C = 1$, which is also accurately verified by our data as shown in Fig. 2. This proves that the formula Eq.(9) is essentially providing a complete analytic form for the leading behavior of the block-entropy scaling in arbitrary dimensions for systems

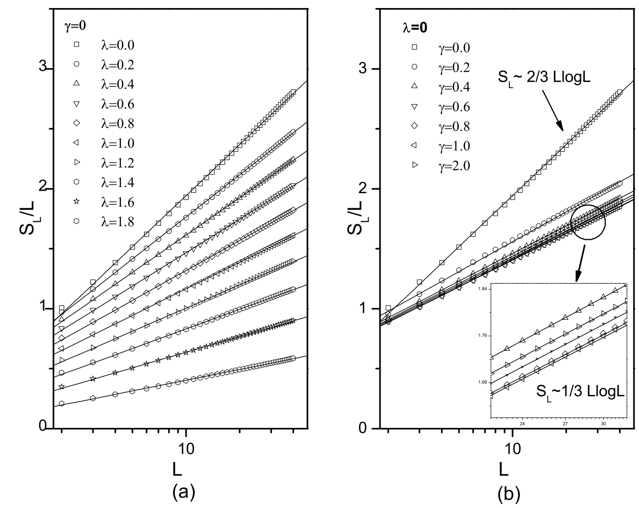

FIG. 2: Scaling of the block entropy S_L in $d = 2$ for $\gamma = 0$ (left panel) and $\lambda = 0$ (right panel). The solid lines correspond to fits according to the formula $S_L = \frac{C}{3}L\log_2(L) + BL + A$.

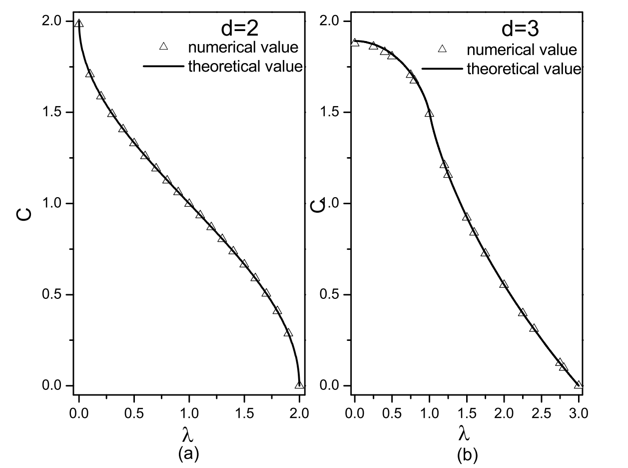

FIG. 3: λ-dependence of the C coefficient in Eq.(1) in $d = 2$ and $d = 3$. The values extracted from fits to our numerical data are compared with the predictions of Ref. 16. In $d = 2$, the exact form of $C(\lambda)$ can be obtained, which is equal to $\frac{2}{\pi}cos^{-1}(\lambda - 1)$

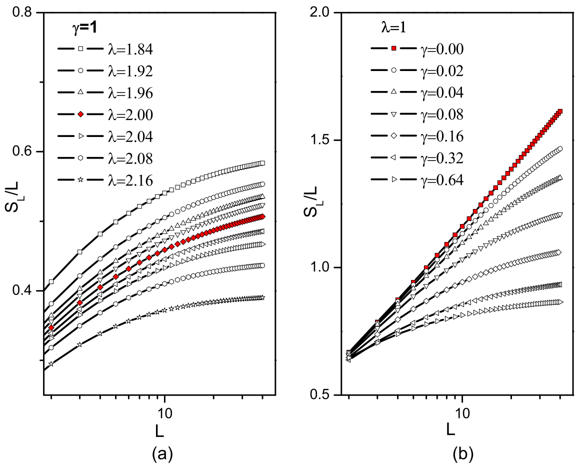

FIG. 4: Scaling of the block entropy S_L in $d=2$ for $\gamma=1$ (left panel) and $\lambda=1$ (right panel).

with a finite Fermi surface.

We then turn to the other two phases, II and III. Two scans through these phases, at fixed $\gamma=1$ and at fixed $\lambda=1$ are shown in Fig. 4. We observe that logarithmic corrections are *absent* in both, and only sublogarithmic corrections are possible. For $\{\lambda \geq d, \gamma=0\}$ $S_L=0$ identically, and the state is not entangled. While the area law is expected to hold in the non-critical phase III, it is surprising to observe it enforced also in the critical phase II, which has a diverging correlation length. This clearly reveals that the connection between block-entropy scaling and correlation properties is not as straightforward as in $d>1$.

Our results for the entanglement behavior, co-dimension, density of states and correlation properties are summarized in Table I. A crucial difference between the two critical phases I and II is the co-dimension $\bar{d}$, and the density of states at the ground state energy. We have $\bar{d}=1$ and $g(0)>0$ in the phase I, which shows logarithmic corrections to the area law, whereas $\bar{d}=2$ and $g(0)=0$ in the phase II, in which the area law is verified up to sublogarithmic corrections. It is therefore tempting to conjecture that a codimension $\bar{d} \leq 1$ or, alternatively, a finite density of states at the ground state energy $g(0)>0$ is a *necessary condition* for critical phases in $d>1$ to show violations of the area law. For the fermionic system under consideration, $\bar{d}=1$ requires the existence of a finite Fermi surface, which is the basic assumption of the proof of area-law violation in Refs. 15, 16. This conjecture would generalize the results for $d=1$, where the co-dimension can only take the value $\bar{d}=1$, and only critical phases with $g(0)>0$ have been explored in the literature.

Further investigations in systems with $d>1$ are clearly needed to confirm this picture, and to clarify whether more severe violations of the area law are possible in presence of infinitely degenerate ground states or in systems with a fractal Fermi surface [15]. During the completion of this manuscript we became aware of Ref. 24 whose results are in full agreement with the ones reported in our work.

	S_L	$\bar{d}$	$g(0)$	$\langle c_i^\dagger c_j \rangle$
Phase I	$\sim (\log_2 L) L^{d-1}$	1	>0	power-law decay
Phase II	$\sim L^{d-1}$	2	0	power-law decay
Phase III	$\sim L^{d-1}$	d	0	exp. decay

TABLE I: Summary of the entanglement scaling properties, co-dimension, density of states and decay of correlations in the three phases of the model Eq.(2) in $d=2,3$.

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